Annals of Nuclear Energy 211 (2025) 110962

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Uncertainty quantification for severe-accident reactor modelling: Results and conclusions of the MUSA reactor applications work package

S. Brumm [a,*], F. Gabrielli [b], V. Sanchez Espinoza [b], A. Stakhanova [b], P. Groudev [c], P. Petrova [c], P. Vryashkova [c], P. Ou [d], W. Zhang [d], A. Malkhasyan [e], L.E. Herranz [f], R. Iglesias Ferrer [f], M. Angelucci [f,1], M. Berdaï [g], F. Mascari [h], G. Agnello [h,2], O. Sevbo [i], A. Iskra [i], V. Martinez Quiroga [j], M. Nudi [k], A. Hoefer [l], E.-M. Pauli [l], S. Beck [m], L. Tiborcz [m], O. Coindreau [n], G. Clark [o], I. Lamont [o], X. Zheng [p], K. Kubo [p], B. Lee [q], M. Valincius [r], M. Malicki [s], T. Lind [s], Y. Vorobyov [t], O. Kotsuba [t], M. Di Giuli [u], I. Ivanov [v], M. D'Onorio [w], F. Giannetti [w], T. Sevon [x]

[a] European Commission, Joint Research Centre (JRC), Westerduinweg 3, 1755 LE Petten, The Netherlands
[b] Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtzplatz, 1, 76344 Eggenstein-Leopoldshafen, Germany
[c] Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences (INRNE-BAS), Tzarigradsko Chaussee 72, 1784 Sofia, Bulgaria
[d] CNPRI, 21/F, Science and Technology Building, Shangbuzhong Road, Futian District, Shenzhen, China
[e] BEL-V, Rue Walcourt 148, 1070 Anderlecht, Belgium
[f] Nuclear Safety Research Unit, Department of Energy, CIEMAT, Avda. Complutense 40 Edificio 12-P0-13 28040 Madrid, Spain
[g] CNSC, 280 Slater Street, Ottawa, ON K1P 5S9, Canada
[h] ENEA, Via Martiri di Monte Sole 4, Bologna 40129, Italy
[i] Energorisk LLC, Off. 141, 7 Simii Steshenkiv Str., Kyiv 03148, Ukraine
[j] Energy Software S.L., ENSO, Catalunya 13, Taradell 08440 Barcelona, Spain
[k] EPRI, 1300 West WT Harris Blvd, Charlotte, NC 28262, United States
[l] Framatome GmbH, Paul-Gossen-Str. 100, 91052 Erlangen, Germany
[m] Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH, Schwertnergasse 1, 50667 Köln, Germany
[n] IRSN, Centre de Cadarache, B.P. 3 – 13115 Saint-Paul-lez-Durance Cedex, France
[o] Jacobs, 305 Bridgewater Place, Birchwood Park, Warrington WA3 6XF, United Kingdom
[p] Japan Atomic Energy Agency (JAEA), 2-4, Shirakata Shirane, Tokai, Naka, Ibaraki 319-1195, Japan
[q] Korea Atomic Energy Research Institute (KAERI), Daedeokdaero 989-111, Yuseong, Daejeon 34057, South Korea
[r] Lithuanian Energy Institute (LEI), Breslaujos Str. 3, 44403 Kaunas, Lithuania
[s] Paul Scherrer Institut (PSI), Forschungsstrasse 111, CH-5232 Villigen PSI, Switzerland
[t] SSTC NRS, 03142, 35-37 V. Stusa Street, Kyiv, Ukraine
[u] Tractebel ENGIE, Severe Accident Group, Avenue S. Bolivar 34-36, Brussels, Belgium
[v] Technical University of Sofia (TUS), 1000 Sofia, 8, St. Kliment Ohridski Blvd., Bl. 12, Bulgaria
[w] Sapienza University of Rome, DIAEE Corso Vittorio Emanuele II 244, 000186 Rome, Italy
[x] VTT Technical Research Centre of Finland, Kivimiehentie 3, Espoo, Finland

* Corresponding author.
E-mail addresses: stephan.brumm@ec.europa.eu (S. Brumm), fabrizio.gabrielli@kit.edu (F. Gabrielli), victor.sanchez@kit.edu (V. Sanchez Espinoza), anastasia.stakhanova@kit.edu (A. Stakhanova), pavlinpg@inrne.bas.bg (P. Groudev), petia@inrne.bas.bg (P. Petrova), pivryashkova@inrne.bas.bg (P. Vryashkova), oupingwen@cgnpc.com.cn (P. Ou), zhangwencheng@cgnpc.com.cn (W. Zhang), albert.malkhasyan@belv.be (A. Malkhasyan), luisen.herranz@ciemat.es (L.E. Herranz), rafael.iglesias@ciemat.es (R. Iglesias Ferrer), michela.angelucci@ing.unipi.it (M. Angelucci), mounia.berdai@cnsc-ccsn.gc.ca (M. Berdaï), fulvio.mascari@enea.it (F. Mascari), giuseppe.agnello04@unipa.it (G. Agnello), aes69@ukr.net (O. Sevbo), andriy.iskra@ukr.net (A. Iskra), victor.martinez@ensobcn.com (V. Martinez Quiroga), mnudi@epri.com (M. Nudi), Axel.Hoefer@framatome.com (A. Hoefer), Eva-Maria.PAULI@framatome.com (E.-M. Pauli), sara.beck@grs.de (S. Beck), livia.tiborcz@grs.de (L. Tiborcz), olivia.coindreau@irsn.fr (O. Coindreau), graeme.clark@jacobs.com (G. Clark), iain.lamont2@jacobs.com (I. Lamont), zheng.xiaoyu@jaea.go.jp (X. Zheng), kubo.kotaro@jaea.go.jp (K. Kubo), leebh@kaeri.re.kr (B. Lee), mindaugas.valincius@lei.lt (M. Valincius), mateusz.malicki@psi.ch (M. Malicki), terttaliisa.lind@psi.ch (T. Lind), yy_vorobyov@sstc.ua (Y. Vorobyov), ol_kotsuba@sstc.ua (O. Kotsuba), mirco.digiuli@tractebel.engie.com (M. Di Giuli), ivec@tu-sofia.bg (I. Ivanov), matteo.donorio@uniroma1.it (M. D'Onorio), fabio.giannetti@uniroma1.it (F. Giannetti), tuomo.sevon@vtt.fi (T. Sevon).
[1] Present address: University of Pisa, Italy.
[2] Present address: Università degli Studi di Palermo, Italy.

https://doi.org/10.1016/j.anucene.2024.110962
Received 4 April 2024; Received in revised form 8 September 2024; Accepted 1 October 2024
Available online 11 October 2024

Nomenclature

AC	Alternative Current
AM	Accident management
ASTEC	Severe Accident code ASTEC
AV	Auxiliary Variable
BE	Best Estimate
BEPU	Best Estimate Plus Uncertainty
BWR	Boiling Water Reactor
CANDU	Canadian-design PWR
CET	Core Exit Temperature
CFVS	Containment Filtered Venting System
CSS	Containment Spray System
DAKOTA	Uncertainty Quantification tool DAKOTA
DBA	Design Basis Accident
DCIS	Direct Cavity Injection System
EFPD	Effective Full Power Days
ELAP	Extended Loss of AC Power
FoM	Figure of Merit
FW	Feedwater
FP	Fission Product
HL	Hot Leg
HPCF	High-Pressure Core Flooder
KONVOI	German-design PWR
LHS	Latin Hypercube Sampling
LOCA	Loss-of-Coolant Accident
LB-LOCA	Large-Break Loss-of-Coolant Accident
MAAP	Severe Accident code MAAP
MB-LOCA	Medium-Break Loss-of-Coolant Accident
MC	Monte Carlo
MELCOR	Severe Accident code MELCOR
MUSA	Management of Uncertainties and Severe Accidents
NPP	Nuclear Power Plant
PDF	Probability Density Function
PORV	Pilot-Operated Relief Valve
PPORV	Pressurizer Power Operated Relief Valve
PWR	Pressurized Water Reactor
RAVEN	Uncertainty Quantification tool RAVEN
RB	Reactor Building
RCP	Reactor Cooling Pump
RCS	Reactor Cooling System
RPV	Reactor Pressure Vessel
SA	Severe Accident
SAM	Severe Accident Management
SAMG	Severe Accident Management Guidance
SBO	Station Black-Out
SB-LOCA	Small-Break Loss-of-Coolant Accident
SG	Steam Generator
SGTR	Steam Generator Tube Rupture
SL	Surge Line
SRCC	Spearmańs Rank Correlation Coefficient
SRV	Safety Relief Valve
ST	Source Term
SUSA	Uncertainty Quantification tool SUSA
TDAFW	Turbine Driven Auxiliary Feed Water
UA	Uncertainty Analysis
UP	Uncertain (Input) Parameters
UQ	Uncertainty Quantification
URANIE	Uncertainty Quantification tool URANIE
VVER	Russian PWR
WP	Work Package
WW	Wet well

Partner organisations in WP5 of the MUSA project

BelV	BelV
CIEMAT	Centro de Investigaciones Energeticas, Medioambientales Y Tecnologicas
CNPRI	China Nuclear Power Technology Research Institute Co. Ltd.
CNSC	Canadian Nuclear Safety Commission
ENEA	Agenzia Nazionale per le Nuove Tecnologie, L'Energia e lo Sviluppo Economico Sostenibile
Energorisk	Limited Liability Company Energorisk
ENSO	Energy Software S.L.
EPRI	Electric Power Research Institute Inc
FRAMATOME	Framatome GmbH
GRS	Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH
INRNE	Institute of Nuclear Research and Nuclear Energy – Bulgarian Academy of Sciences
IRSN	Institut de Radioprotection et de Sûreté Nucléaire
JACOBS	Jacobs Solutions Inc.
JAEA	Japan Atomic Energy Agency
JRC	European Commission Joint Research Centre
KAERI	Korea Atomic Energy Research Institute
KIT	Karlsruher Institut für Technologie
LEI	Lietuvos Energetikos Institutas
NINE	NINE Nuclear and Industrial Engineering SRL
PSI	Paul Scherrer Institut
SAPIENZA	Universita degli Studi di Roma la Sapienza
SSTC	State Enterprise State Scientific and Technical Center for Nuclear and Radiation Safety
TRACTEBEL	Tractebel Engineering
TUS	Technical University of Sofia
VTT	Teknologian tutkimuskeskus VTT Oy

A R T I C L E I N F O

Keywords:
Nuclear reactor
Severe accident
Modelling
Uncertainty quantification
MUSA
Source term

A B S T R A C T

The recently completed Horizon-2020 project "Management and Uncertainties of Severe Accidents (MUSA)" has reviewed uncertainty sources and Uncertainty Quantification methodology for assessing Severe Accidents (SA), and has made a substantial effort at stimulating uncertainty applications in predicting the radiological Source Term of reactor and Spent Fuel Pool accident scenarios.

The key motivation of the project has been to bring the advantages of the Best Estimate Plus Uncertainty approach to the field of Severe Accident modelling. With respect to deterministic analyses, expected gains are avoiding adopting conservative assumptions, identifying uncertainty bands of estimates, and gaining insights into dominating uncertain parameters. Also, the benefits for understanding and improving Accident Management were to be explored.

The reactor applications brought together a large group of participants that set out to apply uncertainty analysis (UA) within their field of SA modelling expertise – in particular reactor types, but also SA code used (ASTEC, MELCOR, MAAP, RELAP/SCDAPSIM), uncertainty quantification tools used (DAKOTA, SUSA, URANIE, self-developed tools based on Python code), detailed accident scenarios, and in some cases SAM actions. The setting up of the analyses, challenges faced during that phase, and solutions explored, are described in Brumm et al. ANE 191 (2023).

This paper synthesizes the reactor-application work at the end of the project. Analyses of 23 partners are presented in different categories, depending on whether their main goal is/are (i) uncertainty bands of simulation results; (ii) the understanding of dominating uncertainties in specific sub-models of the SA code; (iii) improving the understanding of specific accident scenarios, with or without the application of SAM actions; or, (iv) a demonstration of the tools used and developed, and of the capability to carry out an uncertainty analysis in the presence of the challenges faced.

A cross-section of the partners' results is presented and briefly discussed, to provide an overview of the work done, and to encourage accessing and studying the project deliverables that are open to the public. Furthermore, the partners' experiences made during the project have been evaluated and are presented as good practice recommendations.

The paper ends with conclusions on the level of readiness of UA in SA modelling, on the determination of governing uncertainties, and on the analysis of SAM actions.

1. Introduction

Numerical simulation tools are widely used in the nuclear community to assess the behaviour of Nuclear Power Plants (NPP) during postulated accidents including Severe Accidents (SA). The modelling of Design Basis Accidents (DBA), and thus essentially of thermal–hydraulic phenomena, has long ago been extended to Best Estimate Plus Uncertainty (BEPU) modelling, owing to the fact that many experiments exist to identify uncertainty sources and to validate results, see e.g. (CFR, 1996) or (IAEA, 2008). For SA, the situation is more complex: while a large base of experiments exists that supports modelling different phenomena of SA, few integral effects experiments and data from SA are available for support. Even so, the community has turned towards exploring the BEPU approach for improved SA modelling and uncertainty quantification (UQ). The MUSA project has picked up this initiative with the goal of reviewing the foundations, involving a large community, and demonstrating reactor and spent fuel applications.

The basis of the method applied in this paper draws on contributions from the past 80 years. In 2006, Helton (Helton et al., 2006) published a review of sampling-based methods for uncertainty and sensitivity analysis, covering input sampling, propagation and results presentation that covers essential sources of the method. (Glaeser, 2008) proposes to combine the analysis with the order statistics of Wilks (Wilks, 1941) that offers establishing uncertainty limits for a randomly distributed measurement. Instead of working with measured dimensions of fabricated items, (Glaeser, 2008) applies Wilks' method to the sampled distribution of a Figure Of Merit (FOM) created by propagation of uncertain inputs and parameters through a computer code. As an extension of Wilks, Wald's method (Wald, 1943) establishes a formula for the necessary number of samples when tolerance limits for more than one FOM are sought. (Porter, 2019) provides a critical analysis of the underlying statistics when using the Wilks formula in this context, including a derivation, analytical and statistical verification, and a broad discussion.

More publications on the development of the statistical method are referenced in the papers above, but go beyond the code-application nature of the current paper. UA has been applied to SA, but most of the UQ-studies were performed for specific SA-phenomena. Only some of them contained an uncertainty quantification where the key figure of merit is the radiological source term into the environment. Tolerance limits for ST releases following a severe accident were established for a French 1300 MWe PWR (Chevalier-Jabet et al., 2014) and then, for different NPP and different accident scenarios (Ghosh et al., 2021). Other approaches towards applying UA to SA include (Zheng et al., 2016) where the computing effort as a major practical problem is countered by (1) using factor screening to only include input variables that the FOM is sensitive to, and (2) creating surrogate, fast-running models for part of the overall model. (Wang et al., 2022) looks at Wilks' methodology for a Loss-of-Coolant Accident (LOCA) in a Nordic BWR, but focusses on hydrogen production and the timing of vessel failure as FOM rather than ST and ex-vessel phase.

Preliminary work in the reactor applications Work Package (WP) has been published (Brumm et al., 2023). Key aspects of that work were (i) setting-up of the analysis, including the selection of SA sequences and the development of a reference input deck; (ii) practical challenges ranging from the coupling of SA code and Uncertainty Quantification (UQ) tools and the robustness of simulations in the different codes, to dealing with the requirements of computing power; and, (iii) some first results of the analysis. In particular, (Brumm et al., 2023) provides the tables that show exactly reactor types, accident scenarios, SA codes etc. used, for all participants in the WP. As such, it is necessary to consult for a full picture of results presented here. Major insights identified in the preliminary work are the need for optimising resources; the need for expert judgement in selecting the size and details of an analysis, and critically reviewing results; and the avoiding of code crashes, whose handling can compromise the applicability of the mathematical framework of UA.

This paper describes the reactor applications outcome of the MUSA project (Herranz et al., 2021) that was funded under the EU research programme Horizon-2020. The set-up of the exercise, the choices of partners, and challenges found early in the project, are detailed in (Brumm et al., 2023) and are briefly recalled in Section 2 of this paper. For a structured presentation of results in Section 3, the analyses of the many project partners are divided into four categories according to their main goal and aspiration. Good working practices identified are proposed in Section 4, and are followed by conclusions and proposals of further work.

It should be noted that this article can only provide an overview of the project work and outcomes. The partners' work is described in more detail in the appendix of (MUSA deliverable D5.1, 2023).

2. Partners' results

Twenty-three partners carried out and reported work within the reactor applications WP, with some coordination and guidance, but still largely independently. For orientation, Table 1 shows reactor types and initiating events investigated. Where a combination of two events was used, the partner is mentioned in both columns.

For the sake of clarity, the different contributions have been ordered into different categories of analysis according to the goals that they have aimed at achieving. Five categories are proposed for the analyses, to provide some structure for presenting the work carried out:

- analyses that aim at establishing the uncertainty of ST estimates to the fullest extent offered by the SA code;
- analyses primarily oriented at investigating and improving sub-models of the SA code;
- analyses focussing on an accident scenario, and using UA to highlight some features, without including Severe Accident Management (SAM) actions

- analyses focussing on an accident scenario, and using UA to highlight some features, but including SAM actions
- analyses that are mainly testing uncertainty methodology, investigating results produced and how to visualize them.

In all categories, choosing ST FOMs with a high radiological impact was a requirement of the MUSA project. As said before, many details of the set-up of the different analyses can be consulted in the first part of the work (Brumm et al., 2023).

2.1. Full BEPU analysis aimed at achieving a global view of the ST FOM

These analyses are characterised by

- a large number of Uncertain modelling Parameters (UP) that safely covers all important uncertainties across the modelling;
- a well-founded characterization of the UP by means of their Probabililty Density Function (PDF);
- a large number of simulations. This is here assumed to be at minimum sufficient to determine the two-sided tolerance interval (probability content of 95 %, confidence level of 95 %) statistics according to the Wilks' non-parametric method (Wilks, 1941), which corresponds to 93 computations;
- other measures to avoid bias, and check for bias, of the estimated FOM distribution. Failed computations are an example of such other source of bias.

Within MUSA, such analyses were put forward for the case of an unmitigated Extended loss of AC Power (ELAP) in Large-Dry Containment PWR, called scenario P1 in (EPRI, 2021); Table 2 provides metadata of the case that indicate how the first 3 of the 4 points above are met.

With the analyses already concluded at an early stage in the project, the CsI release to the environment with uncertainty bands, as the main ST FOM, was already published in (EPRI, 2021). Distributions of Auxiliary Variables (AV), like the time of containment failure, underline that some transients exist that do not lead to containment failure within the 48 h time window simulated.

Finally, the sensitivities to UPs that were analysed for all FOM and AV are dominated by model form uncertainty that decides which one of alternative sub-models is employed in a simulation, see Fig. 1. CsI release as a key figure of interest is most associated with the enabling of a model for Corium sideward relocation within the core (Boolean parameter ISIDRL) and with calculating, or not, mass and energy transfer between gases and pools in the containment (Boolean parameter IHTGPL). The true model variable GSHAPE that accounts for non-spherical aerosols in coagulation and settling calculations is only third in terms of correlation with the CsI release; the steel solidus temperature TSCS is fourth. This underlines how model-form information is without question key to understanding and improving accident modelling. However, it is a valid point that the model form should be known when running the UA, e.g. through a preparatory analysis step; in this way, the weaker impact of ordinary model parameters could be avoided to be blurred. See (Table 3).

Table 1
Key axes reactor type/scenario of the partners' analyses.

	ELAP	SBO	LB-LOCA	MB-LOCA	c-SGTR
PWR Gen III		KAERI	CNPRI		KAERI
PWR Gen II	EPRI	CIEMAT, ENEA, ENSO, IRSN, KIT& Framatome, PSI, Tractebel	BelV	GRS, KIT& Framatome	PSI
VVER		Energorisk, INRNE, TUS, SSTC	Energorisk, INRNE, TUS		
BWR		Jacobs, JAEA, LEI, Sapienza, VTT	LEI		
CANDU		CNSC	CNSC		

2.2. Analyses focussed on submodels

These analyses are characterised by

- selecting all potentially significant UP in the submodels investigated;
- a well-founded characterisation of the UP by means of their PDF;
- a large number of simulations, as defined in the previous section;
- other measures to avoid bias, and check for bias, of the estimated FOM distribution. Failed computations are an example of such other source of bias.

Goal of these analyses is the detailed investigation of how uncertainties in specific sub-model parameters affect ST uncertainty. Due to this focus, there is no concern for missing important uncertainties in other parts of the overall model, and hence, the result is not a generally valid uncertainty quantification.

Noting the complexity of the simulation, IRSN decided to focus its Station Black-Out (SBO) study on epistemic uncertainties resulting from a lack of knowledge in the models of iodine chemistry and aerosol transport in the containment. As the only partner in the project, IRSN explored an UA focussed on the containment phase of the accident, and thus uncertainty propagation not starting from accident initiation. To reach this goal, (i) the input data deck was built to run ASTEC Fission Product (FP) transport (SOPHAEROS module) computations for the containment; boundary conditions (amount and speciation of FP entering the containment) and containment conditions (temperature, pressure, dose rate and flow rate) were provided by a reference all-modules computation. Further, (ii) two key boundary conditions were set as UP (fraction of gaseous iodine at the break; size of aerosols entering into the containment).

IRSN reports an important reduction in the computing effort that requires one base case simulation from the initiating event, plus 100 uncertainty simulations of the containment phase. The proposed method entails reading transient data of the base case calculation as boundary conditions; a certain error is introduced, since these data are only available for time instants when the output has been saved. Fig. 2 indicates that the containment simulation overestimates iodine release predicted by the all-modules simulation.

Fig. 3 highlights the all-modules base case, left, and percentiles of the total Iodine mass release that have been calculated with the BEPU analysis. Submodel uncertainties lead to an uncertainty band of considerable width at 120 h. It is recalled that this result assumes that no model uncertainties exist outside the submodel of interest and thus in other parts of the model, and cannot claim to be universally valid.

Figs. 1 and 2 (right) show that the release to the environment is a two-stage process, with initially leakages taking place and, after about 40 h into the accident, the Containment Filter Venting System (CFVS) opening. The sensitivity analysis highlights (not displayed here) that the first phase is dominated by FP particle properties, while the longer-term containment phase uncertainty is ruled by the choice, assumed random,

Table 2
Metadata for full BEPU analyses.

	No. UP	UP-PDFs	Submodels[1]	No. runs/ crashed/ recovery	Transient end	SA code
EPRI	232	mixed	all	500/ 0/ –	48 h	MAAP

[1]Nomenclature in all tables of Section 3: AT – aerosol transport, FPT – fission product transport, FPR – fission product release, IC – iodine chemistry, CF – core failure, IBC – initial or boundary conditions, MP – material properties, CONT – containment, ENV – environment, IV – in-vessel.

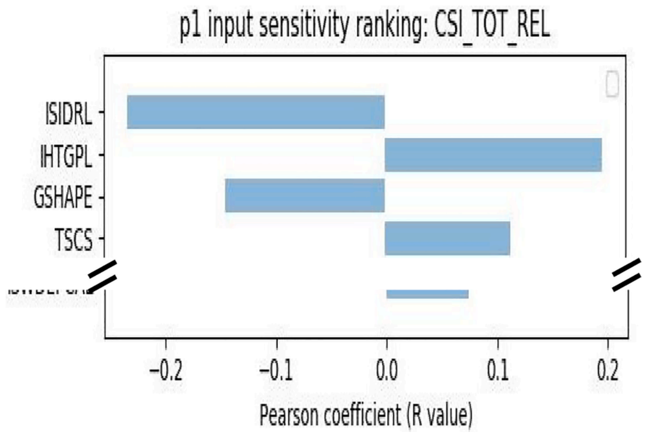

Fig. 1. (From Figs. 8-112 in (Epri, 2021)), Scenario P1: Sensitive input parameters for the maximum fraction of CsI released to the environment. Here, just the 4 most sensitive are shown.

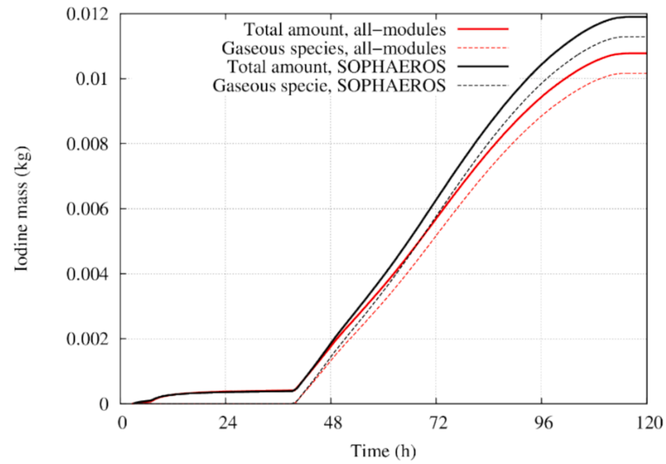

Fig. 2. Evolution of the iodine mass released in the environment for the all-modules computation and for the SOPHAEROS computation [IRSN].

Table 3
Metadata for analyses focussed on sub-models.

	No. UP	UP-PDFs	Submodels[1]	No. runs/ crashed/ recovery	Transient end	SA code
IRSN	43	mostly uniform	IC, AT in CONT	100/ 0/ –	120 h	ASTEC
GRS	81	mixed	FPT	100/ 0/ restart	5.6 h	AC[2]
ENEA	8	mixed	AT	130/ 14/ abandon	27.8 h	MELCOR

whether a model for washing of the walls is used, and by the CH_3I radiolysis in the gaseous phase. It is noted that the switch for the washing submodel is a model-form parameter.

GRS carried out a simulation of a Medium Break LOCA + SBO scenario in a KONVOI PWR, with uncertainties focused on the FP transport model that includes FP behaviour in the containment. No thermo-hydraulic input parameters were assumed as uncertain, the aim of this choice being to evaluate the models directly responsible for the FP behaviour without the undoubtedly present effect of different thermo-hydraulic conditions. Fig. 4 (left) displays the evolution of Iodine aerosols in the containment; upon the beginning of core damage, iodine aerosols in the order of kilograms are released into the containment, where the bigger part of them is deposited. The uncertainty range of this result is large. In the time frame studied, the release to the environment in Fig. 4 (right) is leakage of airbound FP. With thermo-hydraulic uncertainty absent, results show variation only from the time when FP transport rules the accident evolution.

Uncertainties in the environmental release of Iodine were found to be significantly associated with 5 UP, judging by the correlations shown in Fig. 5. The coefficients exceeding an absolute value of 0.2, and in the order of significance, are:

- Agglomeration particle shape factor (GAMMA, #13 of the UP defined by GRS).
- Particle collision efficiency (#14).
- Dynamic particle shape factor (CHI, #12).
- I_2 dissolution from paint after I_2 deposition (#53).
- Pre-factor of reactor constant k13 – second hydrolysis step (#31).

These clear associations make an interesting comparison with the work of other MUSA partners where a wider spectrum of uncertainties was selected and where it was suspected that correlations of FP transport model parameters and FOM where hidden by more dominant uncertain parameters, including SAM actions uncertainties.

ENEA ran the analysis of an unmitigated SBO in a generic PWR-900, where the initiating event of loss of offsite AC power was assumed to coincide with the unavailability of all diesel generators and the independent failure of the Turbine Driven Auxiliary Feedwater (TDAFW), Reactor Coolant Pump (RCP) seals and accumulators. To develop the reference case transient of 100,000 s duration, a MELCOR model of the reactor was used.

Eight aerosol-related "constants" in the model were selected as uncertain input parameters, and the peak of aerosol mass in suspension in the containment's atmosphere taken as FOM for the statistical analysis, see Fig. 6 (left).

This study demonstrates the flexibility in defining meaningful time dependent FOMs other than the mostly selected releases at a certain time or event in the accident transient. The peak of aerosol mass in suspension can be regarded as expressing a hazard potential that would reach the environment in the worst case of loss of the containment function.

Fig. 6 (right) displays the scatter plot of the selected FOM against the aerosol agglomeration shape factor GAMMA, which showed a significant correlation with the FOM.

The three applications in this section focus on aerosol modelling in different SA codes, and agree in the result that aerosol agglomeration, and the model parameter quantifying it, is the effect that the FOMs are most sensitive to. There is further agreement in the results of IRSN and GRS that several aerosol particle parameters, and aerosol interaction with the containment wall, correlate with the FOM: this is an opening into understanding and working on the submodel. Even so, it must be remembered that the MUSA exercise is not a benchmark and that most choices of the 3 partners – type of reactor, scenario, list and PDF of UP, FOM, etc. – diverge.

2.3. *Analyses focussed on scenarios without accident management*

Six MUSA partners carried out analyses that can best be described as being focussed on a certain accident scenario. In this case, the UA is expected to help better understand which of the set of selected uncertain parameters is affecting the scenario most.

Analyses are characterised by:

- Careful set-up of the scenario (usually well known);
- In most cases a medium number of UP;
- Typically, a number of simulations oriented at the Wilks 95/95 criterion, i.e. about 100, which is a large effort for most SA codes and computing environments.

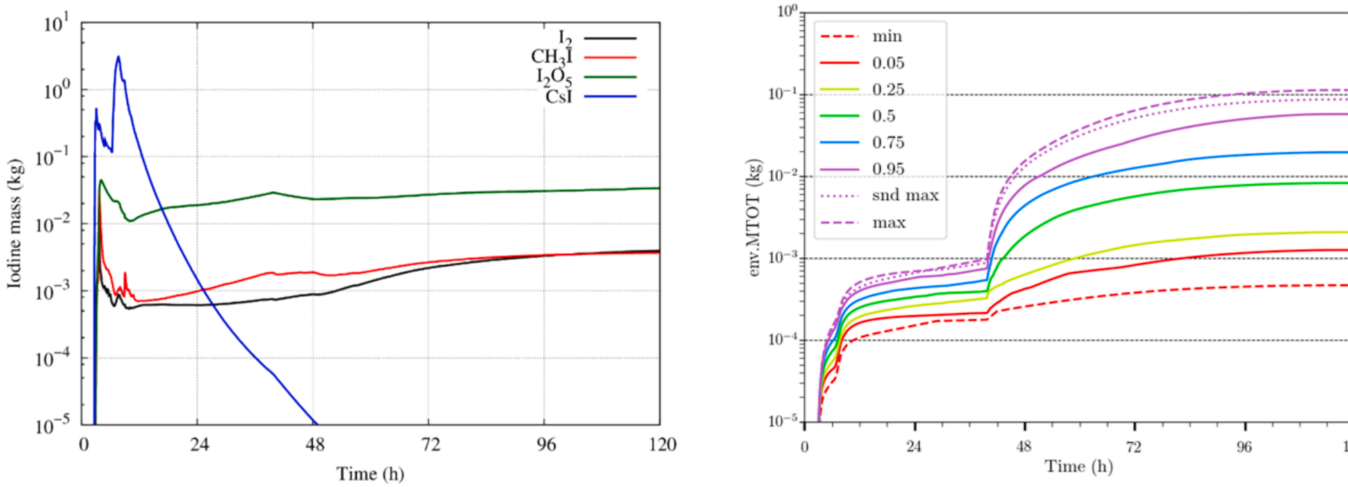

Fig. 3. Evolution of Iodine released. Base case airborne Iodine species (masses are related to the iodine element) in the containment (left); from the BEPU analysis, various percentiles of total Iodine mass released to the environment (right) [IRSN].

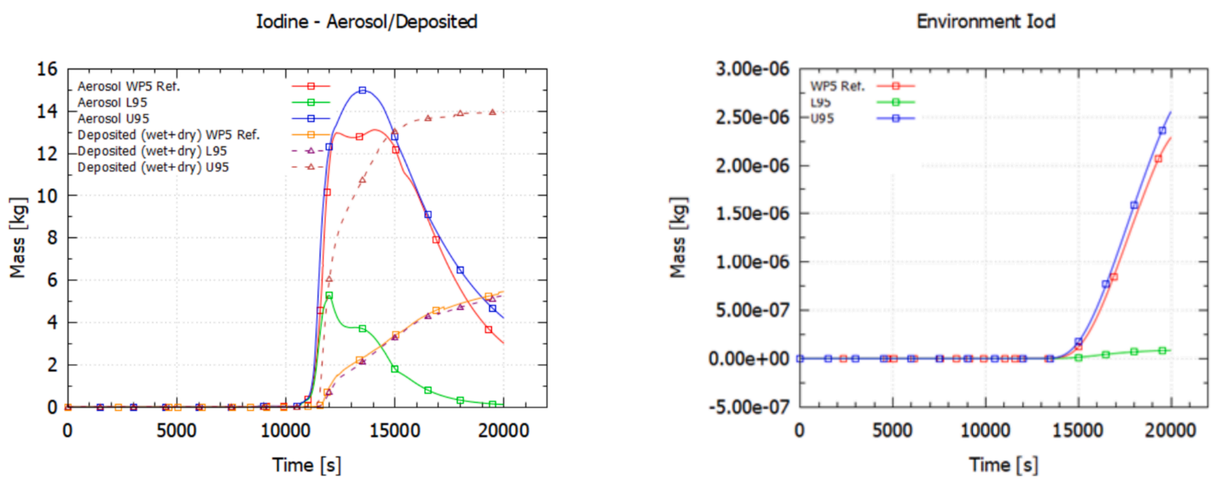

Fig. 4. Uncertainty bands for Iodine in the containment (left); and, Iodine leakage to the environment (right) [GRS].

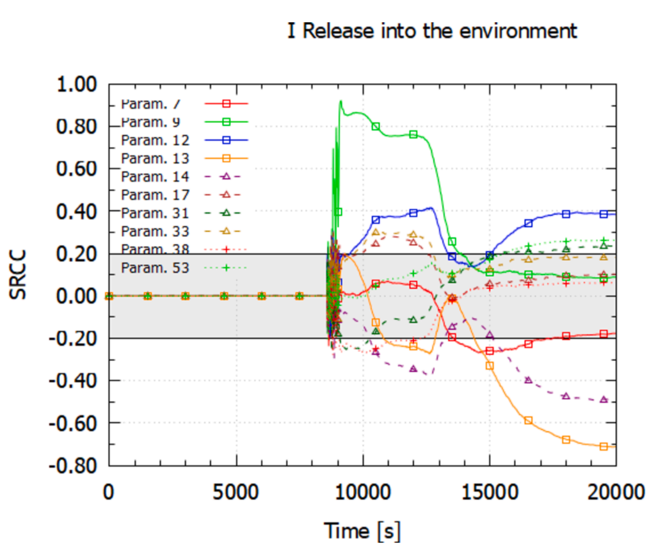

Fig. 5. Spearman Rank Correlation Coefficients between Iodine release to the environment and UP [GRS].

CIEMAT analysed an unmitigated SBO scenario with batteries lasting for 6 h and ensuring availability of measurement and control, and in particular TDAFW. Within 48 h, the scenario takes the plant through a sequence of events including a consequential steam line break of one Steam Generator (SG), hot leg creep rupture, Reactor Pressure Vessel (RPV) break and eventually containment break. Uncertainty was attached to parameters selected from the core initial inventory; the FP release model (CORSOR-BOOTH); models for fuel and cladding failure; and, aerosol characterization.

Main conclusions of this study are that the UA improves the understanding of the best estimate of the 3 FOM – Iodine, Caesium and noble gas releases to the environment – by adding an uncertainty band – and that the onset of the release is associated to significant uncertainty. Fig. 7 shows the containment failure time and major release lies within 34 h – 40 h for the completed simulations, with two outliers; the Iodine release at the end of the simulation lies between 86 and 95 % of the initial inventory. The Best Estimate (BE) base case turns out to be on the non-conservative side of the analysis.

The iodine release to the environment is found to be most strongly associated with the molecular iodine inventory, and to a lesser extent, with the scale coefficients in the CORSOR-BOOTH model and the particle shape factor for aerosol agglomeration.

CNPRI: A Large Break LOCA scenario with unavailable safety injection systems was simulated; despite core melt, the ex-vessel and

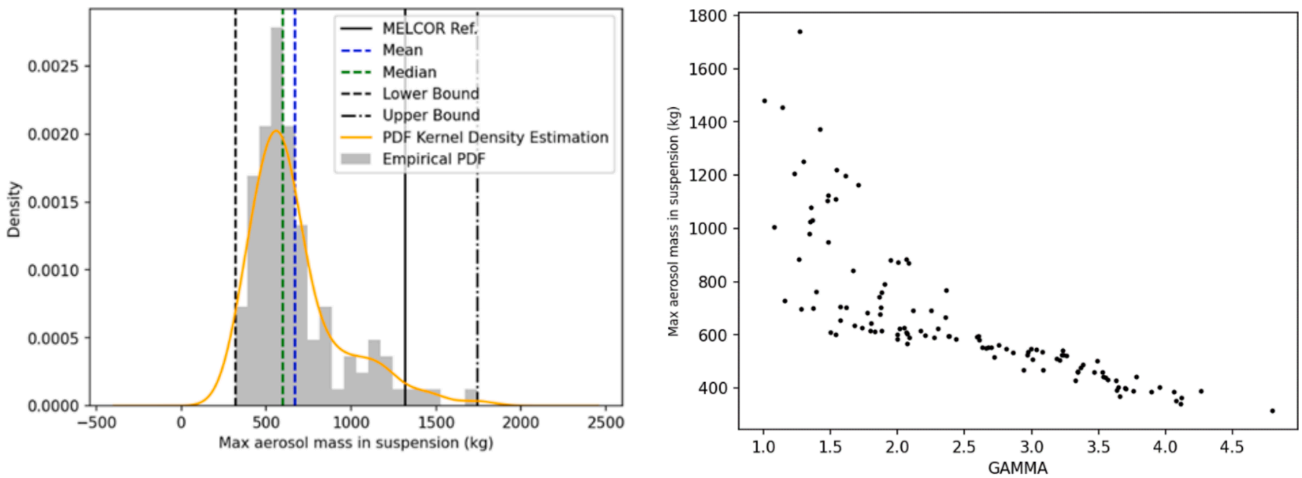

Fig. 6. Empirical PDF of the FOM "peak value of the aerosol suspended mass in the containment's atmosphere" (left). Scatter plot of the same FOM over values of GAMMA (right) [ENEA].

containment cooling systems in the Gen. III reactor prevent RPV failure and containment break. Five parameters related to sources and sinks of iodine in the containment were defined as uncertain; they are displayed in Table 5. In this analysis, the UPs significantly contributing to uncertainty in the iodine release to the environment are (i) the gaseous iodine mass release fraction from primary circuit to containment and (ii) a residual ratio that determines how much of the aerosols deposited on walls in the containment may be washed down due to draining and condensed water films, and transported into the lower compartments.

KIT & Framatome applied different post-processing tools to a common set of propagated data. The organisations had a particular interest in the selection of fuel burn-up as an uncertain parameter, for which the ORIGEN ARP tool was employed to evaluate a library of fuel inventories each 30 effective full power days for a total of 328 EFPD. This is a comprehensive study in the sense that it has looked at an MB-LOCA base scenario and two variations with aggravated circumstances, and at the situation with CFV as SAM action (though without uncertainty in that action). The simulation lasted until basemat failure.

Fig. 8 compares containment pressure in the three base cases: it rises very quickly to over 4 bar and then takes a transient reflecting assumptions of each case. Fig. 9 shows the release of Iodine to the containment (left) and the environment (right), together with the calculated uncertainty band for the basic MB-LOCA scenario.

Monte-Carlo simulations of the considered MB-LOCA scenario were used to establish correlations between the UP and the ST (Stakhanova et al., 2023). High correlations during the whole accident were observed for the containment leakage, while the fuel burnup only has a high correlation at the beginning of the accident when the FP release from the fuel pellets starts. Parameters describing the aerosol behaviour are important at later stages of the accident.

Simulations of the considered MB-LOCA scenario were also used to establish correlations between the radioactive ST and plant data measured during a SA, such as the dose rate in the containment and the annulus. The simulation data were then used as training data for a time series prediction algorithm based on the MOCABA data assimilation framework (Hoefer et al., 2015). It has been demonstrated that the developed algorithm is generally suitable to perform real-time ST predictions during SA using plant data measured during the accident (Pauli et al); (Stakhanova et al., 2023). This makes it possible to use this algorithm within real-time accident predictor modules at NPPs.

PSI: An SBO scenario was analysed where a stuck-open Safety Relief Valve (SRV) in one SG leads to Steam Generator Tube Rupture (SGTR) some hours into the scenario. Feed water (FW) is recovered for an interval of about 8 h and helps mitigate the SGTR; after losing FW again, the accident transient leads to vessel failure. In the simulated time, the

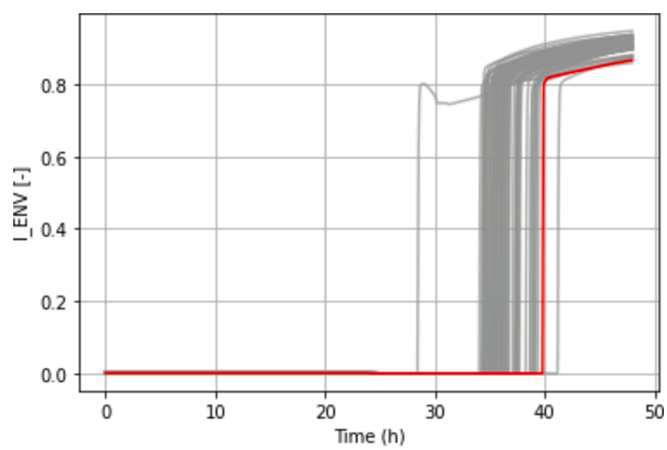

Fig. 7. Iodine release to the environment, with the BE base case marked by the red line [CIEMAT].

containment maximum pressure is not reached, and FP release to the environment takes place through containment leakage only.

In addition to the release of Cs, CsI and CsM to the environment, retention of these isotopes in the damaged SG was used as a FOM; ensemble evolutions for CsI are displayed in Fig. 10. These data suggest a significant release of CsI to the environment, with a median value, at the end of the simulation, of about 24 % initial inventory in terms of Iodine, and a wide uncertainty band of about 23 % (left). At the same time, about 7 % of CsI are still retained in the SG, with an uncertainty band of about 4 % (right). This is extra insight into uncertainty and trends of FP localization.

In addition to the focus on the scenario, PSI invested much effort into analyzing the sources of code crashes, checking for systematic error, and mitigating them by re-running, adapting the minimum time step.

Sapienza: A BWR SBO scenario with stuck-open PORV and wet well (WW) venting was modelled. Venting was applied as a fixed (no uncertainty) SAM action, triggered by the containment pressure exceeding 5.2 bar. Fig. 11 shows the importance of the wet well for trapping CsI.

The mass of CsI released at 55 h into the transient, as the primary FOM, was found to be most strongly associated to the "temperature to which oxidized fuel rods can stand in the absence of un-oxidized Zr in the cladding" and to the aerosol dynamic shape factor.

The venting action significantly reduces the standard deviation of CsI trapped in the WW. The UA demonstrated the significant impact of uncertain parameters on hydrogen production and CsI release in a BWR

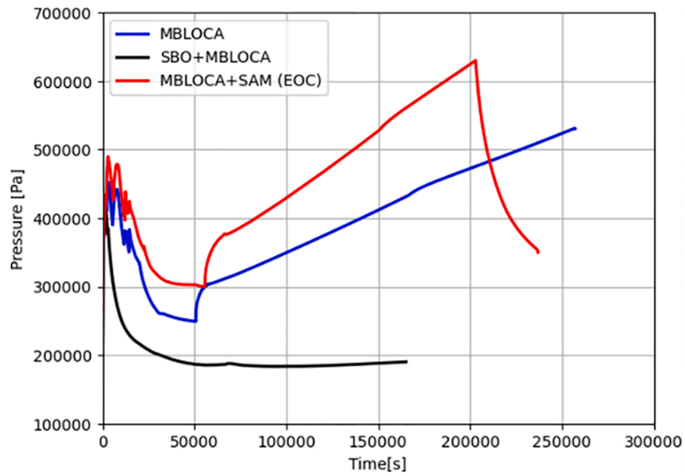

Fig. 8. Pressure in the containment (left) and in the annulus (right) [KIT & Framatome].

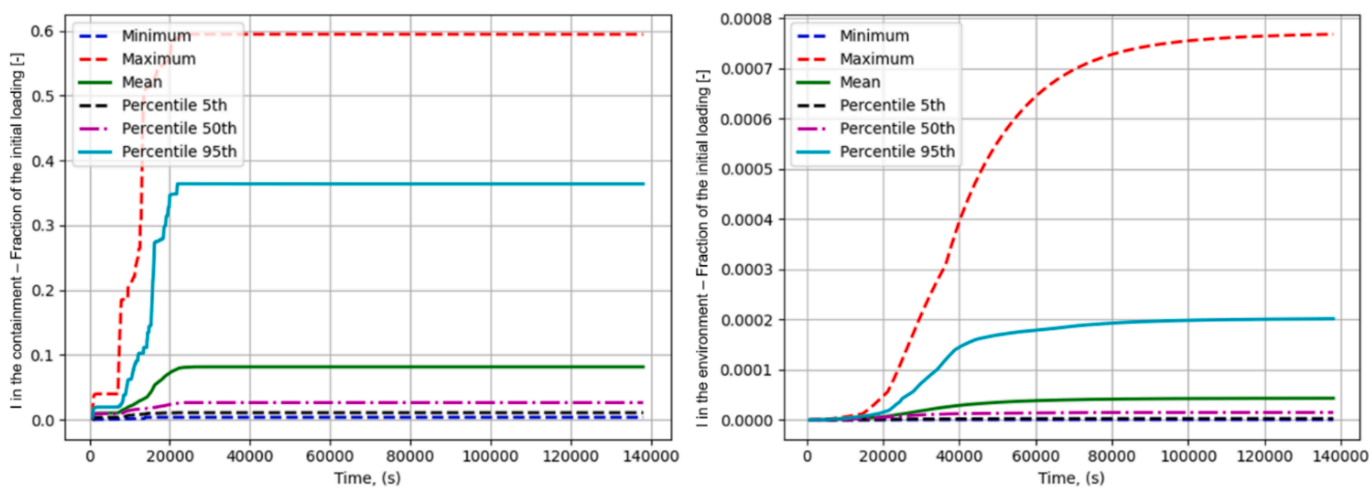

Fig. 9. Statistics of the evolution of total mass of iodine in the containment and in the environment as fraction of the total amount in the initial core loading in the ASTEC MB-LOCA scenario [KIT & Framatome].

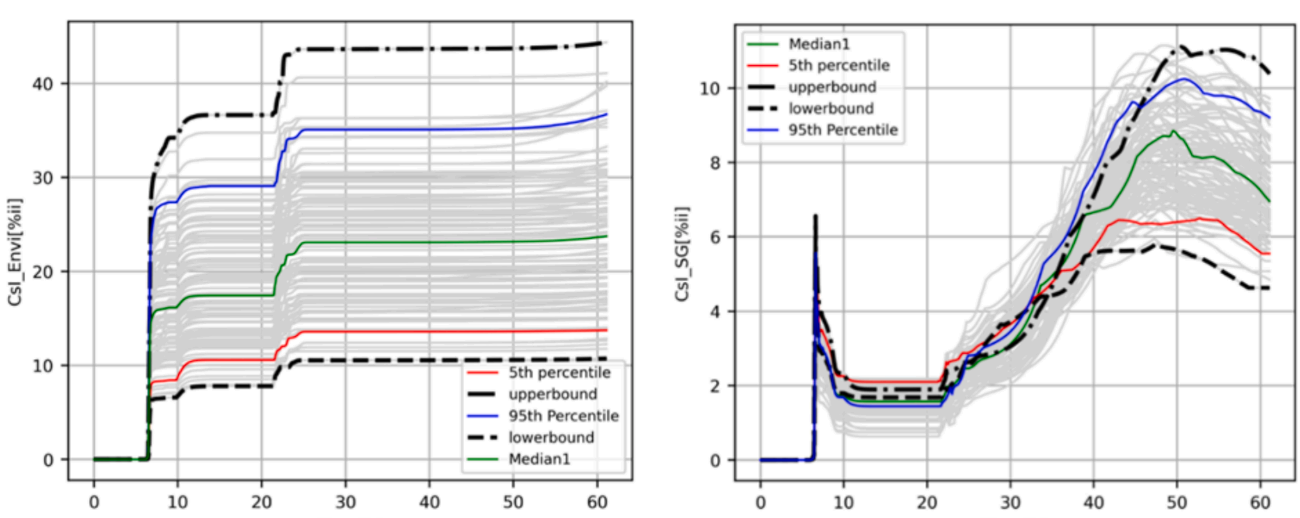

Fig. 10. Ensemble evolution: CsI release to the environment (left) CsI retention in damaged SG (right) [PSI].

during a SBO scenario, revealing wide variability in outcomes. Strong correlations between core degradation parameters and FOM were identified, emphasizing the complexity of interactions.

The cases in this section have been grouped together for being based on carefully selected accident scenarios and using UA to investigate particular aspects of that scenario, like: how the predicted CsI release (timing and magnitude) in a complex accident scenario strongly depends on model uncertainties, and a best estimate base case is clearly non-conservative (CIEMAT); a detailed comparison of 3 MB-LOCA scenarios, with feeding a plant-prediction algorithm (KIT-Framatome); an investigation of the impact of FP retention in the SG in a SGTR scenario (PSI); and, the importance of the wet well for trapping CsI in a BWR (Sapienza).

The analyses produce insights into the UP most associated with FOM variations, as further detailed in (MUSA deliverable D5.1, 2023). However, due to the significant differences between the analyses, the dominant parameters found are essentially not shared between the different cases. Finally, it has to be stressed that most partners saw a substantial number of unsuccessful simulations (see Table 4), i.e. that the requirement for a strict statistical interpretation was not met.

2.4. Analyses focussed on scenarios with accident management

This definition covers the case of scenarios with SAM actions are related to uncertain parameters, where the analyses are expected to provide feedback on the impact of that action and could provide hints as to how to improve SAM and the way it is modelled.

In terms of objective, these analyses are still focussed on scenarios, like those in Section 2.3.

JAEA: A Fukushima-like scenario initiation has been investigated, where the modelling is integrating Containment Filter Venting System (CFVS) decontamination factors for aerosols and vapour, and the timing of alternative firewater injection, as uncertain parameters. The sensitivity analysis for the ST release fraction, see Fig. 12 (right), shows the highest degree of association with (1) the firewater injection timing that leads in many cases to stopping the accident, and thus zero FP release; (2) decay heat; (3) the particle slip factor in the aerosol model; and, CFVS decontamination factor for aerosols.

The plot of iodine release fractions for all accident transients in Fig. 12 (left) illustrates these results: with the firewater injection starting time t_{fi} uniformly distributed in the interval [34.72 h, 48.61 h], few cases of $t_{fi} < 40$ h lead to important iodine release – the SA is stopped. If the water injection arrives too late, then the containment is pressurized and the CFVS will be triggered. The iodine release magnitude shown in Fig. 12 is directly impacted by the uncertainty on the decontamination factor. The result confirms the effectiveness of early re-flooding.

KAERI: A consequential SGTR event initiated by an SBO was simulated. As typical for this sequence, the core starts to overheat and lose liquid after the SG have dried out. Overheated steam in the primary, and the persisting high pressure, can lead to creep rupture of hot leg (HL) and/or PRZ surge line (SL); furthermore, reverse flow patterns in the SG can lead to SGTR; see Fig. 13 (left) for an illustration. This complex situation was subjected to an uncertainty analysis by assigning uncertainty ranges to 3 key thermo-hydraulic parameters and to the cross sections of potential line and tube breaks; furthermore, the timing of a SAM action, i.e. operating the Atmospheric Dump Valve, was defined as uncertain.

The results of 210 successful simulations fall into different scenario evolutions with consequential failures, see Fig. 13 (right). In 42 % of the cases, SGTR happens first; in 22 % of cases, SGTR happens after HL/SL rupture. However, in 35 % of cases, HL/SL ruptures but SGTR never takes place. With respect to ST FOM, this is a bifurcation scenario: SGTR bypasses the containment and leads to FP releases, while the containment tightness is never challenged in the scenario and in the simulated time frame.

This case is instructive for its illustration of a challenging scenario, and for demonstrating that bifurcation can happen and needs to be dealt with in the BEPU analysis.

SSTC: In an SBO scenario for a VVER, it was explored how the uncertain number of available PORVs (1, 2 or 3) impacts the evolution of the accident; among 43 uncertain model parameters, this number showed the largest association with the amount of Cs released to the environment by the end of the simulation. Fig. 14 (left) shows PORV availability (Par 38), HTC between debris and water (Par 29) and aerosol dynamic shape factor (Par 2) as the uncertainties most strongly impacting Cs class release.

The PORV influence was further investigated by running 3 more UA where the number of available PORVs was fixed to 3, 2 and 1: every available PORV adds to the cross section available for depressurization; on these grounds, the speed of the depressurization and the re-flooding by hydro accumulators will gradually change, and a logical expectation would have been that the Cs release is also showing a clear trend towards less release for larger cross section. Fig. 14 (right) suggests that this is not the case. The largest Cs release is found for 2 available PORVs, not one. This is taken as a reminder of the complexity of severe accident scenarios.

Tractebel: This work is standing out by the choice of UP; in addition to 10 parameters mainly in the modelling of core failure and radionuclide behaviour, triggering conditions of 3 management actions were set as discrete random variables relative to switching to SAMG (time

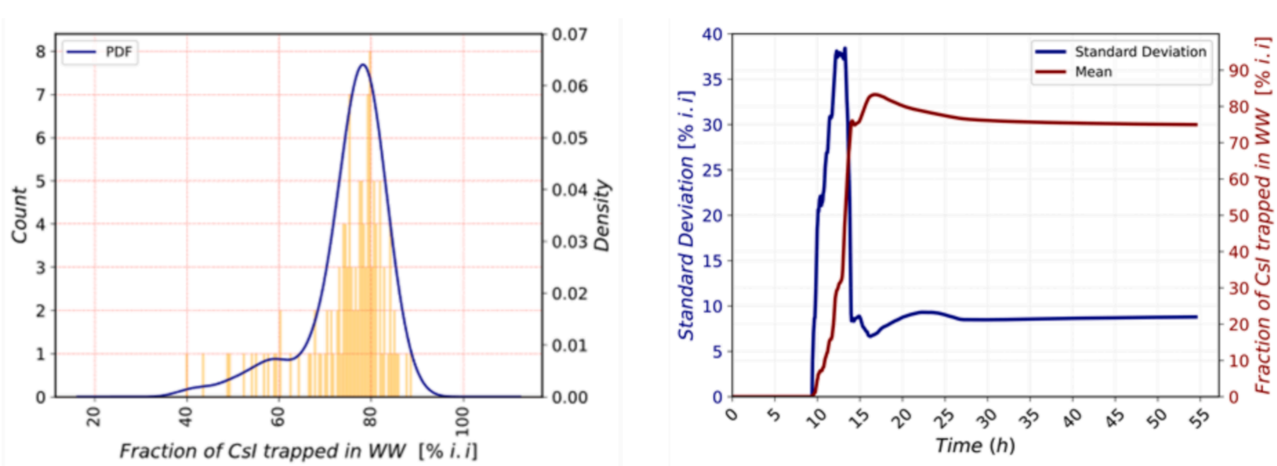

Fig. 11. Fraction of CsI trapped in the WW. Empirical distribution at the end of the sequence (left) and evolution of standard deviation and mean value over the sequence (right) [Sapienza].

Table 4
Metadata for analyses focussed on scenarios without accident management.

	No. UP	UP-PDFs	Submodels[1]	No. runs/ crashed/ recovery	Transient end	SA code
CIEMAT	24	Triangular, unif.	AT, FPR	93/ 35/ abandon	48 h	MELCOR
CNPRI	5	Uniform	IC	100/ 26/ abandon	168 h	ASTEC
KIT&Framatome	16	Mixed	FPR, CF, AT, fuel burn-up	3x300/ (21/6/12)/ abandon	Basemat failure, ≈ 55 h	ASTEC
PSI	17	Uniform	CF, AT	100/ 0/ restart	61.1 h	MELCOR
Sapienza	21	Mixed	CF, AT	200/ 63/ abandon	55 h	MELCOR

Table 5
UP, their ranges, and their correlation (Pearson coefficient) with computed gaseous Iodine releases to the environment [CNPRI].

Uncertain Parameter	Variation Range	Correlation with Iodine released to the environment
I_2 mass release fraction from primary circuit	0 ~ 0.5	0.962
Residual fraction of washing effect	0 ~ 1	0.698
Adsorption rate of I_2 for painted dry surfaces	10^{-5} ~ $2*10^{-3}$	0.167
pH value in IRWST	3 ~ 7	−0.116
Additional dose rate in IRWST	0 ~ 2	0.090

$t_{CET=650C}$ at which the Core Exit Temperature (CET) reaches 650 °C), and time t_{VF} of vessel failure.

PPORV opening time [s]	$t_{CET=650C}$ + [700.,1000., 1200., 2000., 3000., 4000., 5000.]
CSS triggering time [s]	t_{VF} + [0.0, 5000., 10000., 15000., 20000., 25000., 30000., 40000., 1.0E6]
DCIS triggering time [s]	t_{VF} + 1800 + [0.0, 5000.,10000., 15000.,20000., 25000., 30000., 40000., 1.0E6]

Containment filtered venting was also part of the analysis, and here the uncertainty was equally distributed between 5 discrete activation threshold pressures.

CFVS opening pressure [Pa]	[4.0E + 5, 4.5E + 5, 5.0E + 5, 5.5E + 5, 6.0E + 5]

Of all UP, only the Pressurizer Power-Operated Relief Valve (PPORV) opening time and the CFVS opening show strong association with 3 selected FOMs, see Fig. 15. Of the remaining UPs, some show a low degree of correlation. It is not clear whether that low degree of correlation of the UPs in the MELCOR model is due to the fact that no correlation actually exists, or whether uncertainties in other SAM actions dominate and reduce them.

The main conclusion on the SAM actions related to CsI release are:

- Delaying the intervention of the CSS leads to larger CsI release through the Annular Space/containment leakages into the environment. This is due to the fact that sprays' intervention reduces the CsI aerosol suspension time in the Reactor Building (RB) atmosphere;
- Delaying the pressurizer PORV on the other hand reduces the amount of CsI reaching the environment through the RB leakages (time-limited effect up to 100000 s). The reason is that large amount of CsI remains deposited on the surfaces of the Reactor Cooling System (RCS), in the first phase of the transient.
- As the opening pressure of the CFVS increases, the number of venting operations decreases. By postponing the first venting operation responsible for the largest radioisotope release, the cumulative amount of CsI reaching the environment is overall reduced;
- By delaying the manual opening of the three pressurizer PORVs, the deposited mass of CsI in the RCS increases, thus reducing the amount of CsI entering the containment and consequently its release through RB leaks;
- The direct injection of water in the cavity by means of the Direct Cavity Injection System (DCIS) has a negligible effect on the release of volatile FPs. The FPs that remain trapped in the corium are those with low or medium volatility, while almost 95 % of the CsI is released during the core degradation and before the VF;
- The behaviour of Cesium Molybdate and Cs metal are quite different from CsI. This may be related to the different vapor pressure characterizing these Cs compounds, giving them a different volatility and condensation behaviour.

2.5. Analyses focussed on applying UA to SA and identifying issues

MUSA has also seen contributions that do not fit the previously described categories well; they have been driven by a range of goals, like (i) focussing on single effects; (ii) exploring the interpretation of results; (iii) looking at possibilities to navigate limitations in computer hardware and in modelling that is limited to in-vessel phenomena.

Jacobs performed 5 uncertainty quantification studies using a generic Gen III BWR model, with the aim of gaining an understanding of the relative influence of a set of UPs chosen from the WP2 database and

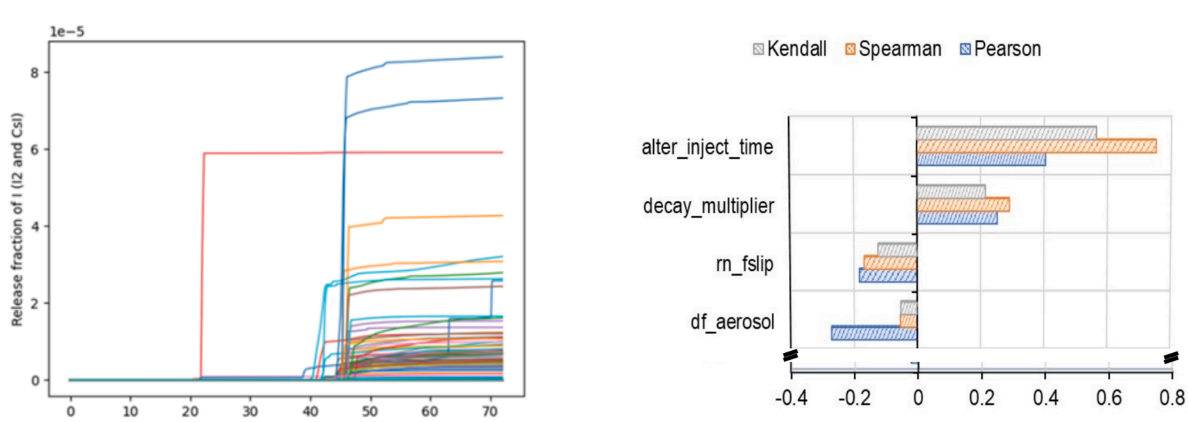

Fig. 12. Iodine release to the environment (left); and, sensitivity analysis between source term release fraction and input parameters, showing just the four most significant correlations (right) [JAEA].

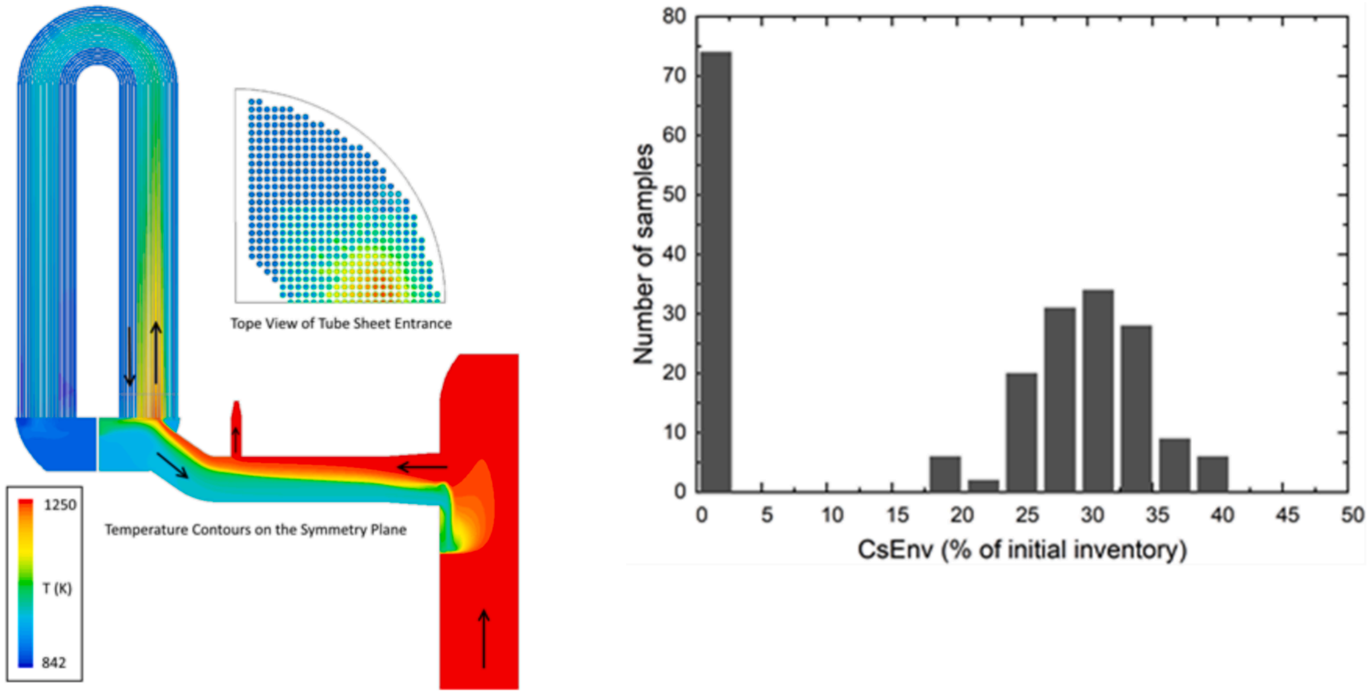

Fig. 13. Natural convection of steam via hot leg and SGTs (left); bifurcated PDF of FOM"Cs released to the environment" (right) [KAERI].

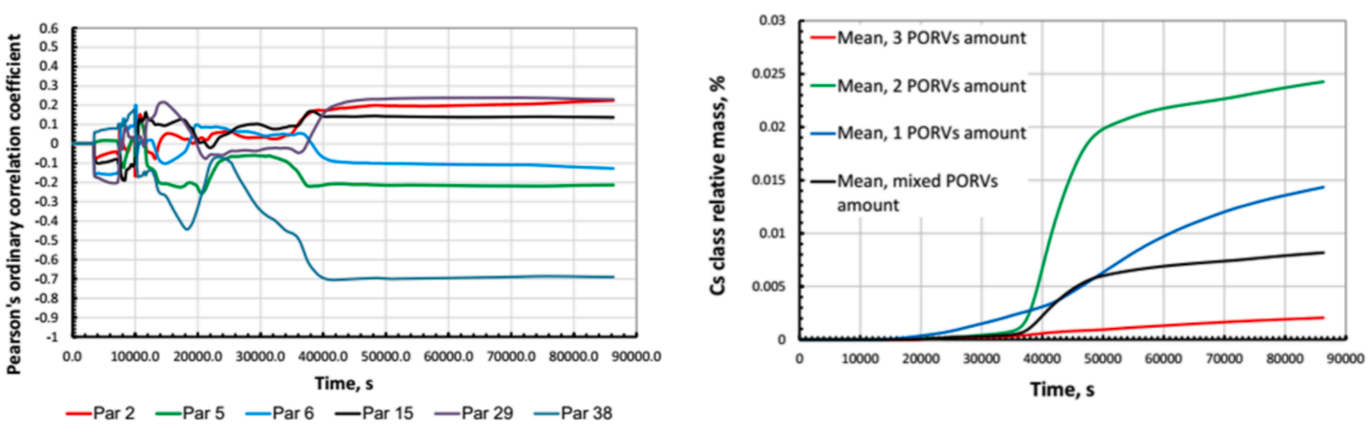

Fig. 14. Cs class release to environment, time-dependent sensitivity analysis (left); Cs release to environment (FOM2) mean value for different number of operable PORVs (right) [SSTC NRS].

uncertainties associated with a SAM action (High-Pressure Core Flooder (HPCF) timing and flow rate) on source term uncertainties, as well as the interaction between them. Identifying the parameters with the strongest influence on FOM uncertainties was not a key objective of this work, hence the number of UPs selected was small.

An aspect in the work worth spotlighting is the exploration of how to deal with frequent code crashes, and how code restart could introduce bias into the calculated output FOM. Jacobs propose an automated mechanism of (i) a local time step reduction shortly before the code crash experienced, and (ii) a restart from scratch. If necessary, this mechanism can be repeated several times.

As a means of testing a potential bias introduced by such frequent restarts, it is proposed to inspect the empirical FOM distribution – see Fig. 16, where the outputs for the different number of restarts have been plotted in different colours. In the given case, abandoning simulations rather than restarting would have led to bias.

The immediate approach to dealing with crashed simulation includes the need to plot the values of UP and exclude a pattern of values in the failed runs. The approach proposed by Jacobs adds another view on such patterns and could be useful in further work on reducing bias in reactor applications.

VTT demonstrated essential elements of the method by highlighting (i) the benefit of a stable input deck; (ii) how just 22 simulations are required when applying Wilks one-sided criterion with 90 % probability/90 % confidence; and, (iii) and, how testing the statistical significance of correlations, by means of calculating the P-values with the Student's *t*-test, could determine aerosol shape factor and gas-to-particle thermal conductivity ratio as certain regressors in the multiple regression analysis. See (Table 6).

CNSC ran robust simulations with the MAAP/CANDU code. They looked at a LOCA and an SBO and showed differences (i) in uncertainties and sensitivities of the CsI release for these two scenarios; (ii) for a comparison of UP PDFs being all uniform vs. a mixed set of distributions; and, (iii) the effect of doubling the number of simulations from 100 to 200. CNSC used the FOM PDF at different time instants to demonstrate and compare the impact.

INRNE analysed a LB-LOCA/SBO scenario that is mitigated by the recovery of water injection when the CET passes 980 °C. This fast

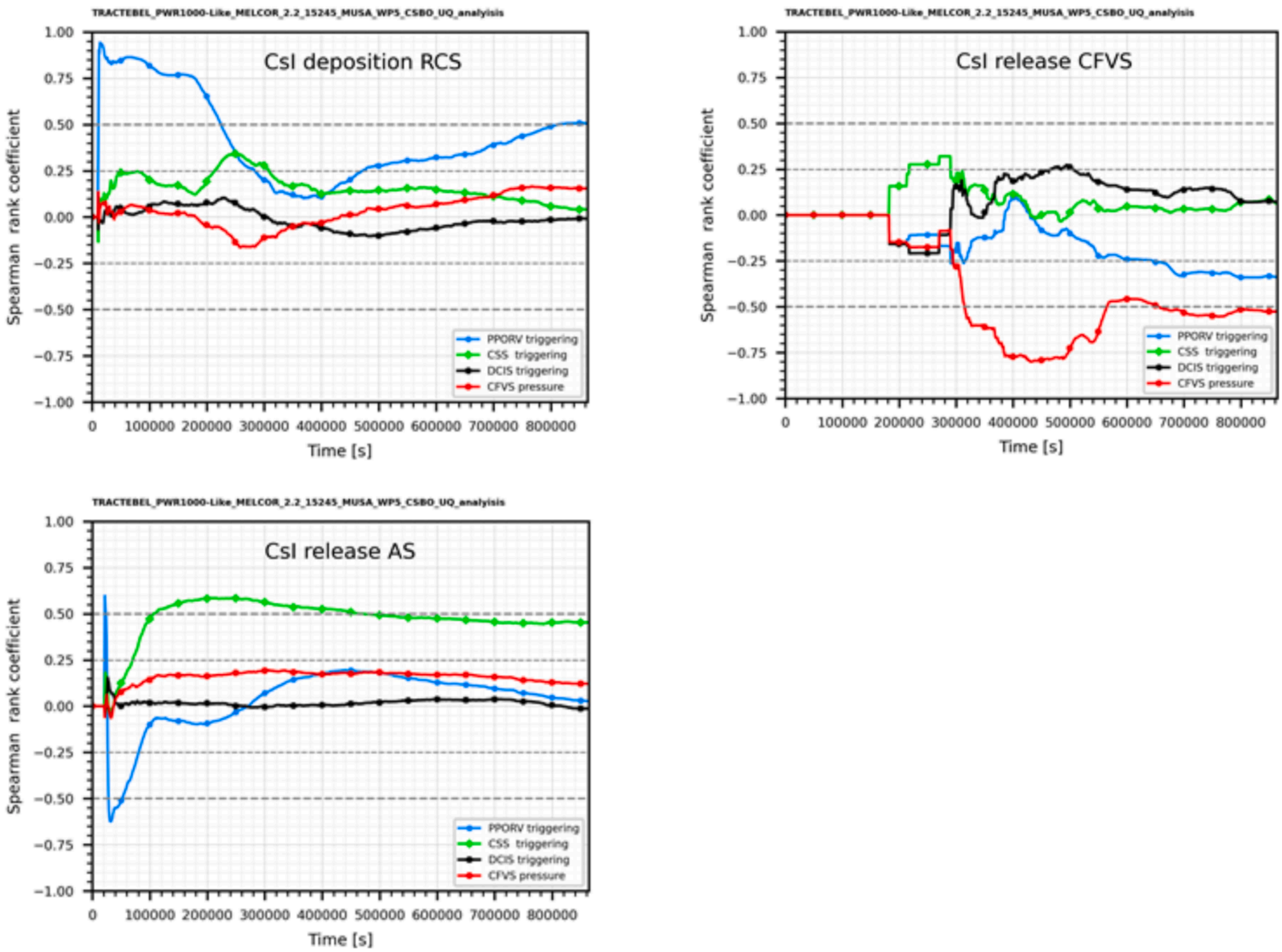

Fig. 15. Spearman rank correlation coefficients for SAM action uncertainties and CsI release. Deposition (top left); release through CFVS (top right); release to the containment Annular Space (bottom left) [Tractebel].

scenario, taking little more than 2300 s, allowed testing most modelling aspects asked in MUSA – FP release, aerosols behaviour, deposition and suspension, and gaseous iodine – while limiting very much the computational effort of 100 simulations.

TUS proposed a similar but less drastic medium break scenario, with the recovery of low-pressure injection after the passing of CET = 650 °C and an operational delay of 1000 s.

LEI took part in the project with the RELAP/SCDAP code that is limited to modelling the in-vessel phase of a severe accident. The harsh LB-LOCA + SBO scenario leads to a fully uncovered core within 50 s; the key FOM is FP (Cs, I) released from the core at the end of the transient, which is the time of the first slump of UO2 to the lower head, at around 3000 s.

ENSO improved the capabilities of RELAP/SCDAP RS3.4 for ST analysis by implementing a Fission Product Transport model and satisfying the Wald criterion to track the uncertainty margins of 3 FOM simultaneously. Results of the UA are proposed to be used as input for ex-vessel simulations with containment codes.

Energorisk looked at very fast scenario, a double-ended guillotine break of Primary Circuit Pipeline (2 x DN850 cold leg) coinciding with an SBO, with FP gap release starting after 170 s; the simulation end time is 1000 s. The UA exercise was carried out according to steps agreed in MUSA and leads to dispersion plots that portray the evolution of FOM in the 59 simulated cases. However, the absence of significant correlations between FOM and UP suggests that there is no knowledge gain on the

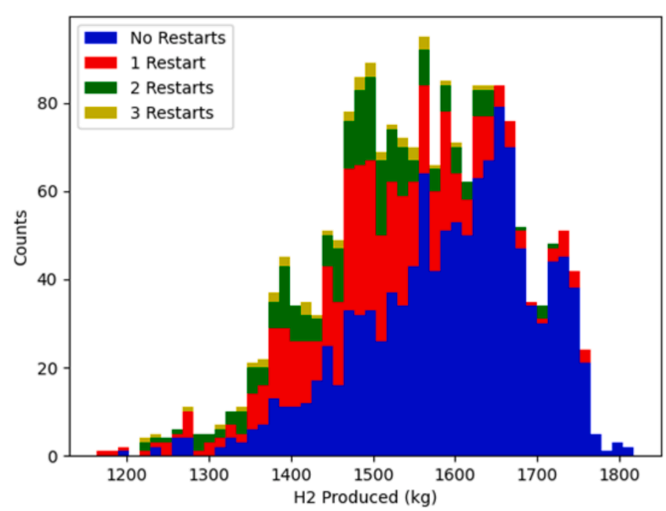

Fig. 16. Mass of Hydrogen (FOM) produced for a study where the timing of activating a high-pressure core flooder was taken as randomly distributed. The results are broken down by the number of time step reductions/restarts required to get the calculation to run to completion [Jacobs].

extreme scenario through the UA.

The scenario analysed by BelV is similar to Energorisk's, a large break LOCA with failure of safety injection; however, the simulation of 24 h of the scenario provides a view of both in-vessel, and part of the ex-vessel, phase. FP release to the environment during the simulation time span is only through containment leakage. At 24 h, the sensitivity analysis shows a weak correlation of Cs release to the environment only with the level of decay heat.

This section has collected applications of UA that have been limited in most cases (but not all) to accommodate the computational facilities and resources that partners could make available, and have focussed on the method itself, on building experience with it and on isolating some of its issues like interpretation of statistics. This content re-affirms that MUSA has also been about training its partners in setting up UA for SA, and about supporting more widespread use in future projects.

3. Good practice recommendations

A key motivation for the focus of MUSA on applications has been the goal to involve the SA community and to create a base of experience that can be shared, and be built upon. Partners' accounts of their challenges and recommendations have been collected (MUSA deliverable D5.1, 2023) and summarised (MUSA deliverable D5.2, 2023).

Before going into the detail, it is necessary to discuss the level of these recommendations. In setting up MUSA, the ambition was to establish "best practice". Looking at the results that have been produced within the project, however, it is clear that the UA application to SA is work in progress; there is a body of experience, but more harmonisation and consolidation is needed to formulate best practice recommendations. That is why this section proposes "good practices" identified in the project. See (Table 7).

3.1. Definition of uncertain model parameters

(CFR, 1996) points out assumptions for the application of Wilks' method when quantifying the uncertainty band of a FOM: (i) all relevant UPs (i.e. affecting the FOM) need to be covered, and (ii) their input probability distributions accurately known. The best practice shown in MUSA is the approach of EPRI, where a large number of 232 UP from all sub-models of MAAP was selected and where a large effort has been made over the past years to build up a database of suitable definitions of model parameter uncertainty. Several other partners (e.g. GRS with 81, SSTC 43 UP) have successfully carried out the analysis with a large number of UP, but have been less exhaustive in terms of sub-models and UP covered.

Several partners focused their analysis on the identification of dominating uncertainties in a sub-model; IRSN, GRS and ENEA have shown that the choice of a large number of UP in the FP transport model – that is closely linked to the ST released to the environment – offers good insight into the modelling.

Point (ii) above has been an active field for partners' investigations. Values and PDFs of these parameter uncertainties have been collected in a database in MUSA (MUSA deliverable D2.2, 2023).

Good practice acknowledged is:

- the impact of accurate and reliable information on model parameter uncertainty for estimating relevant error margins of FOM. Work of EPRI and within MUSA WP2 underlines the need for a sustained effort involving expert knowledge of model developers;
- PDFs, especially normal and lognormal, should be bounded to avoid outliers that could present unphysical values and were found to lead to code crashes.

(Porter, 2019) notes that marginal distributions tend to be too conservative, and that covariant distributions should be preferred. However, this thematic was not addressed.

3.2. Number of samples

The modus operandi evolving here was the use of the Wilks formula, typically 95/95, to indicate the minimum number of samples. Several partners used the LHS with the Wilks method that is proven only for random sampling. This is an incompatibility that has not been addressed strictly in MUSA: first, it has been regarded as having less impact than many other choices in setting up the analysis. But it is also worth further exploring whether the advantageous properties of the LHS method over random sampling favour its continued use.

When code crashes are experienced, the way most used to overcome them was to find out a proper (shorter) time step near the time of the code crash. At the end of MUSA, the most thoroughly investigated method is an automatic local reduction of the minimum time step shortly before and after the registered crash, and a restart form zero of the simulation in question (Jacobs).

3.3. Management of uncertainty quantification

Uncertainty analysis requires multiple runs of the SA simulation, from pasting uncertain parameter values into the input deck, launching the execution, re-launching crashed cases, to assembling output files and analysing the data. At the outset of the project, most partners expected to use available UQ tools for these tasks. However, after experiencing inflexibility of such tools in carrying out all tasks necessary in the particular SA application; limitations to their given functions; and, in a few cases, coupling problems that could not be resolved, the best practice recommended for now is to write dedicated interfaces by means of e.g. the Python programming language. Some partners have gone much further than this and have developed.

- statistical analysis tools (KATUSA by KIT)
- tools that adapt the time step around the time of a simulation crash and restart that simulation (Jacobs)
- procedures and code to deal with thousands of simulations (e.g. EPRI, Jacobs)

3.4. Dealing with the large computing effort

SA modelling is highly complex, with a host of phenomenological models integrated with each other to track what could happen during an accident scenario. The effort of computing a transient is to some degree determined by modelling choices of the user, like the coarseness of

Table 6
Metadata for analyses focused on scenarios with accident management.

	No. UP[1]	UP-PDFs	Submodels[1]	No. runs/ crashed/ recovery	Transient end	SA code
JAEA	12 + 3	Mixed	CF, FPR, AT	340/ 180/ abandon	72 h	MELCOR
KAERI	5 + 1	Mixed	SG and break model	300/ 90/ abandon	48 h	MELCOR
SSTC	40 + 3	Uniform	all	100/ 0/ reduce time step	24 h	MELCOR
Tractebel	11 + 4	Uniform	CF, FPR, AT	111/ 11/ restart[2]	240 h	MELCOR

[1]m+n, with m the number of ordinary UIP in the SA model, and n those related to the SAM action
[2]where restart is unsuccessful, abandon the run.

Table 7
Metadata for analyses focussed on applying UA to SA and identifying issues.

	No. UP	UP-PDFs	Submodels[1]	No. runs/ crashed/ recovery	Transient end	SA code
Jacobs	7 + 2		CF, SAM	4 x 1000/ 10–50 %/ abandon	48 h	MELCOR
INRNE	8	uniform	CF, FPR, other	100/ 0/ –	2300 s	ASTEC
CNSC	10		CF, AT, other	2x 350/ 0/ –	138.9 h	MAAP
VTT	8		AT, IBC	22/ 0/ –	24 h	MELCOR
TUS	5		CF	30/ 1/ abandon	13.7 h	ASTEC
LEI	16		CF,MP in-vessel	100 / 35/ abandon	2700 – 4000 s	RELAP/SCDAPSIM
ENSO	19		CF in-vessel	124/ 24/ time step change	≈10 h	RELAP/SCDAPSIM
ENERGO RISK	8	uniform	CF, AT	59/ 0/ –	1000 s	MELCOR
BelV	22	Mix, 14 unif.	CF, AT	208/ 20/ abandon	24 h	MELCOR

nodalisation; but as has been confirmed in MUSA, it is even more conditioned by the implemented models, which heavily affect both the time step required to compute phenomena and the robustness towards code crashes. While most codes used posed significant challenges as to the sheer time it took to compute the large number of simulations required for UA, and the dealing with code crashes, the fast-running MAAP code knows hardly any challenge of this sort.

This being a major problem in MUSA, partners have spent an effort to develop practical solutions to managing the computing effort. In summary, they recommend to:

- Use adequately powerful computing hardware;
- Create a robust input deck, and test it to demonstrate its stable execution;
- Consider the exclusion of sub-models that lack robustness. This is a key issue of the entire exercise, because this simplification will reduce the quality of modelling the physical phenomenon. In the longer run, such models should be improved in robustness;
- Develop a strategy and a software solution for restarting crashed simulations. For reasons of limitations to resources in the project, most partners chose to abandon crashed simulations. Those who took the effort to recover crashed runs went mostly for reducing the minimum time step shortly before the crash time and restarting the calculation.

Away from the BEPU method itself, there is clearly also an effort spent with managing the huge amount of data produced, particularly when dealing with hundreds or thousands of simulations. Some partners have indicated which parts of the results they extract and save for future reference, but this has not been a point for systematic reporting.

3.5. Plausibility of results

Creating and processing a large number of results risks losing the view over whether results are plausible. It has to be demanded that all the results of an analysis should be understood and should be physically consistent to be considered; if some of the cases in an analysis evolve in a way impossible to explain on physical grounds, either the reasons need be found (numerical or of any other sort) or they should be neglected.

Many partners have realised this common practice by looking at robust and meaningful outputs. Good examples are:

- Horse-hair diagrams plot all accident transients of a target quantity – let's say containment pressure – in one diagram. Knowing the expected evolution, this set of curves is easy to check for its outliers and for where the bulk lies. In many cases, percentiles have been plotted into such diagrams to highlight further features of the data set.
- Input and output values of the set of simulations are also valuable basic information. Collecting all estimates of the FOM and plotting its sampled PDF highlights important information on e.g. distribution shape, bifurcation, etc. and allows conclusions on the character of simulations. Creating a scatter plot of estimates of a FOM against the uncertain values of one input parameter gives an idea of a correlation pattern.

3.6. Consideration of bias

All but the first recommendation in Section 3.4 can introduce bias into the solution. (Porter, 2019) notes that Wilks' method requires to accurately sample the output distribution, and that any significant biases in the output can propagate to the estimate of uncertainty bands. This is an obvious conflict between the theory and the practical solution of challenges faced in the reactor applications: simplification in the modelling, and crashed/ignored simulations are all leading to bias in the empirical FOM distribution.

Recommendations regarding the bias coming from crashed simulations are proposed by Jacobs in (MUSA deliverable D3.3, 2023). By graphically displaying which samples of the empirical output PDF (here for H_2 in containment) have been computed directly or added after 1, 2 or 3 restarts, it is shown that the PDF without restarts is biased; see Fig. 16. In terms of the Uncertainty Band determined by the Wilks method, that bias affects the lower bound of the H_2 estimate, but seems negligible for the upper bound.

With little effort of MUSA going into this issue, it is not so much a best practice, but a recommendation for future work that the quantification of bias be addressed.

3.7. Analysis and improvement of SAM actions

Five MUSA partners have run accident scenarios where uncertainty was attributed to the triggering, and some model parameters, of SAM actions. They have shown that extending the UQ framework to SAM actions is essentially straightforward, no matter whether it is the timing or a parameter defining the quality of the SAM action.

Triggering uncertainties introduced in MUSA have been linked to (i) primary depressurisation by PORVs; (ii) the dumping of secondary-side steam; and, (iii) water injection by core re-flooding, cavity re-flooding, or containment spray. Typically, the uncertainty has been introduced as a random delay of the action after the earliest possible time instant. An example is the opening of PORV after the time instant when the CET is reaching 650 °C and, in the reactor type, mitigation actions prescribed in the SAMG have to be applied. Regarding its impact, the triggering of an action has been found to be typically more significant than quality parameters, e.g. a pumping rate that is more comparable to parameters in the SA model.

The timing of SAM actions is suspected of causing code crashes. This seems plausible considering that the physical impact shortly after triggering should be important, and could require for a short time a smaller than the minimum time step. Such a code crash could be recovered by a local adaptation of the minimum time step, as found in Jacobs' work. This observation needs to be consolidated, and should be regarded as a general observation for now.

The implementation of different SAM actions during the scenario has been explored, and has allowed drawing conclusions on the most effective mitigation (Tractebel, SSTC).

Recommended practices to be mentioned with this work are:

- a realistic scenario of the SAM action(s) taken should be selected, ideally reflecting valid SAMG;
- preliminary testing of the AM to be modelled, to become aware of consequences of the action, including that it might lead to bifurcation or no release at all (Jacobs, KAERI);
- in case of an AM action causing bifurcation, full understanding of the branches' meaning should be achieved (KAERI).

3.8. Statistical analyses

Regarding sensitivity analysis, correlations have been less broadly exploited in MUSA than was originally planned, and the analyses have mostly looked for significant linear correlations. The practice recommended is the computation of p-values for establishing the sample-dependent limit below which a correlation coefficient has a low probability of being significant. This is important information when comparing different analyses with different numbers of simulations.

For the statistics of uncertainty bands it is important to meet the assumptions of the order statistics framework put forward by Wilks (Wilks, 1941), and used and discussed by (Glaeser, 2008); (Porter, 2019). Here, avoiding bias of the sampled empirical FOM distribution is the key objective. This issue has been discussed above, in several sections.

4. Conclusions and further work

Reactor applications have been a focus of MUSA, with the involvement of 25 partner organisations and 30 % of the project's human resources. A broad range of reactor designs, SA codes, uncertainty quantification tools and accident scenarios brought to the exercise by the participants, has helped create a wealth of information on the use of the BEPU method in severe accident modelling.

This paper has aimed at providing a cross-sectional view of the results of participants in the reactor applications work package, from the perspective of key aspects involved in Uncertainty and Sensitivity Analysis. Detailed accounts of each partner's work are provided in the appendix of (MUSA deliverable D5.1, 2023).

At the outset of the project, the goal for the reactor applications WP was formulated as demonstrating the applicability and the level of readiness of uncertainty assessment in the broad range of set-ups presented by different NPPs and different tools investigated by the partners. Also, the results achieved by propagating uncertainties through different integral SA codes were to be assessed using UQ tools, and governing uncertainties were to be determined. These are useful criteria to structure the conclusions.

4.1. Level of readiness of UA in SA modelling

MUSA has demonstrated that the necessary tools are available and can be handled, having first been coupled and tested on the integral core damage experiment Phebus FPT-1, in WP4 of the project, and then used in reactor applications and spent fuel simulations. As a result, a large database of applications has been created, and reports documenting the work made available. The work has also shown the level of preparation and effort required: (i) many of the partners have invested heavily into the coupling of SA code and UQ tools, some even developing Python-based tools to gain flexibility that they missed in available UQ tools. This has been a one-time effort that was underestimated when setting up MUSA; and, (ii) the sheer number of simulations and volume of data, and the dealing with challenging code robustness issues, have been described.

Moreover, there has been a spread of how extensive analyses are, with partners approaches reaching from limiting themselves to the in-vessel part of the accident scenario, to very comprehensive and long-duration scenarios.

Notwithstanding this positive practical outlook, the readiness is also linked to methodological issues. The applicability of the statistical method – and thus strong statements about uncertainty margins – poses strict requirements that are met in BEPU analyses applied to thermo-hydraulic modelling within design-basis-accident analysis, but remain challenging when working on SA. The widespread nature of applications and choices in MUSA has not allowed going much into such issues.

4.2. Determination of governing uncertainties

This goal has guided all contributions made to the work package, but few applications have covered all elements that are required for a full analysis of a particular accident scenario, i.e. a sufficiently complete set of uncertain input parameters; adequate knowledge of these UP; and, a large number of simulation runs, without a significant number of code crashes.

Also, most partners limited their analyses to checking for linear correlations between FP release and the UP, as a consequence of project resources shifting towards the coupling of tools and the uncertainty propagation step. Future work will need to put emphasis on a more thorough look at governing uncertainties and should reach, or go beyond, the standard set in (Ghosh et al., 2021).

4.3. SAM actions

The MUSA proposal set out that uncertainty in innovative AM measures would be considered in addition to initial/boundary conditions and model parameters, and that the SAM impact on the radiological ST prediction would be explored. Five partners defined uncertainty in SAM actions and followed the recommendations of the MUSA End Users' Group to investigate "consequences of injecting water in reactor, cavity or containments, right timing (…) for venting containments through a FCVS." Primary depressurization was also analysed.

On the basis of this small sample of applications, it is concluded that, first and foremost, the BEPU method is readily extended to also include parameter uncertainty related to SAM actions. Given their character of mitigating the accident, and changing or even bifurcating the accident transient, it is of little surprise that SAM action uncertainty has typically been found to dominate FOM uncertainty.

No recommendations for improvement of SAM actions have been made in MUSA, mainly due to the focus on methodic issues. Even so, it has been recognized that BEPU analysis supports an improved understanding of how SAM works in the presence of multiple uncertainties, and this can indeed help improve SAM.

Questions for the investigation of SAM actions in UA remain, like (i) how to best combine the uncertainties in modelling parameters and in SAM actions in an UA; (ii) how uncertainties in "triggering & efficiency" of a SAM action affects uncertainties in the FOMs, and how uncertainties in variables responsible for "triggering" an action affect the efficiency of that action.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Many of the data used have been published in the deliverables of the EU-funded project. Simulation data produced belong to the project partners who should be approached with requests.

Acknowledgements

The MUSA project has received funding from the Euratom research and training programme 2014 – 2018 under grant agreement No. 847441. This paper reflects only the authors' view; the European Commission is not responsible for any use that may be made of the information it contains.

References

Brumm, S., Gabrielli, F., Sanchez-Espinoza, V., Stakhanova, A., Nudi, M., Groudev, P., Ou, P., Herranz, L.E., 2023. Uncertainty Quantification for Severe-Accident reactor modelling: set-up and first results of the Horizon-2020 project MUSA. Ann. Nucl. Energy 191. https://doi.org/10.1016/j.anucene.2023.109919.

10 CFR 50.46, "Acceptance criteria for emergency core cooling systems for light water nuclear power reactors," Appendix K, "ECCS Evaluation Models", to 10 CFR Part 50, Code of Federal Regulations, 1996.

Chevalier-Jabet, K., Cousin, F., Cantrel, L., Séropian, C., 2014. Source term assessment with ASTEC and associated uncertainty analysis using SUNSET tool. Nucl. Eng. Des. 272, 207–218. https://doi.org/10.1016/j.nucengdes.2013.06.042.

EPRI, "Severe Accident Uncertainty Quantification and Analysis Using the Modular Accident Analysis Program (MAAP)", Technical Report 3002020762 (2021). Accessed on https://www.epri.com/research/programs/061177/results/3002020762 on 21/12/2023.

Ghosh, S.T., Esmaili, H., Hathaway III, A.G., Osborn, D.M., Bixler, N.E., Brooks, D., Ross, K.W., Wagner, K.C., 2021. State-of-the-art reactor consequence analyses project: uncertainty analyses for station blackout scenarios. Nucl. Technol. 207, 441–451. https://doi.org/10.1080/00295450.2021.1875737.

Glaeser, H., 2008. GRS method for uncertainty and sensitivity evaluation of code results and applications. Science and Technology of Nuclear Installations 7. https://doi.org/10.1155/2008/798901.

Helton, J.C., Johnson, J.D., Sallaberry, C.J., Storlie, C.B., 2006. Survey of sampling-based methods for uncertainty and sensitivity analysis. Reliab. Eng. Syst. Saf. 91. https://doi.org/10.1016/j.ress.2005.11.017.

Herranz, L.E., Beck, S., Sánchez-Espinoza, V.H., Mascari, F., Brumm, S., Coindreau, O., Paci, S., 2021. The EC MUSA project on management and uncertainty of severe accidents: main pillars and status. Energies 14 (4473), 1–11. https://doi.org/10.3390/en14154473.

Hoefer, A., Buss, O., Hennebach, M., Schmid, M., Porsch, D., 2015. MOCABA: a general monte carlo-bayes procedure for improved predictions of integral functions of nuclear data. Ann. Nucl. Energy 77, 514–521. https://doi.org/10.1016/j.anucene.2014.11.038.

IAEA, "Best Estimate Safety Analysis for Nuclear Power Plants: Uncertainty Evaluation", Appendix 'Definitions'. Safety Report Series No. 52 (2008).

MUSA deliverable D2.2: Major sources of uncertainties during severe accidents in LWR and SFP affecting the ST (2023).

MUSA deliverable D3.3: Best-practice Guidelines of uncertainty quantification performed within MUSA project (2023).

MUSA deliverable D5.1: Results of uncertainty assessment of Source Term released to the environment (2023).

MUSA deliverable D5.2: Best practices for the assessment of Source Term uncertainty when performing severe accident simulations with SAM actions using system codes (2023).

Pauli, E., Hoefer, A., Gabrielli, F., Stakhanova, A., Sanchez-Espinoza, V.H., Prediction of the radiological consequences of a severe accident scenario in a generic Konvoi nuclear power plant", 10th European Review Meeting on Severe Accident research (ERMSAR2022), May 16-19, Akademiehotel, Karlsruhe, Germany.

Porter, N.W., 2019. Wilks' formula applied to computational tools: a practical discussion and verification. Ann. Nucl. Energy 133, 129–137. https://doi.org/10.1016/j.anucene.2019.05.012.

Stakhanova, A., Gabrielli, F., Sanchez-Espinoza, V.H., Hoefer, A., Pauli, E.M., 2023. Uncertainty and sensitivity analysis of the ASTEC simulations results of a MBLOCA scenario in a generic KONVOI plant using the FSTC tool. Ann. Nucl. Energy 192. https://doi.org/10.1016/j.anucene.2023.109964.

Stakhanova, A., Gabrielli, F., Sanchez-Espinoza, V.H., Hoefer, A., Pauli, E.M., 2023. Application of the MOCABA algorithm and the FSTC tool for source term predictions during severe accident scenarios. Ann. Nucl. Energy 184. https://doi.org/10.1016/j.anucene.2023.109703.

Wald, A., 1943. An extension of wilks' method for setting tolerance limits. Ann Math Stat.

Wang, W., Chen, Y., Ma, W., 2022. Application of uncertainty analysis methods to MELCOR simulation of postulated severe accidents in a Nordic BWR. Nucl. Eng. Des. 392. https://doi.org/10.1016/j.nucengdes.2022.111764.

Wilks, S.S., 1941. Determination of sample sizes for setting tolerance limits. Ann. Math. Stat. 12, 91–96.

Zheng, X., Itoh, H., Tamaki, H., Maruyama, Y., 2016. "An integrated approach to source term uncertainty and sensitivity analyses for nuclear reactor severe accidents. J. Nucl. Sci. Technol. https://doi.org/10.1080/00223131.2015.1044262.